# class09

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# 10/27/2021

```
fna.data <- "WisconsinCancer.csv"</pre>
```

```
wisc.df <- read.csv(fna.data, row.names=1)
head(wisc.df)</pre>
```

##		diagnosis ra		<pre>texture_mean p</pre>		${\tt area\_mean}$	
	842302	M	17.99	10.38	122.80	1001.0	
##	842517	М	20.57	17.77	132.90	1326.0	
##	84300903	М	19.69	21.25	130.00	1203.0	
##	84348301	M	11.42	20.38	77.58	386.1	
##	84358402	М	20.29	14.34	135.10	1297.0	
##	843786	М	12.45	15.70	82.57	477.1	
##				ctness_mean con	cavity_mean co	oncave.poir	nts_mean
##	842302	0.11	.840	0.27760	0.3001		0.14710
##	842517	0.08		0.07864	0.0869		0.07017
##	84300903	0.10		0.15990	0.1974		0.12790
##	84348301	0.14	250	0.28390	0.2414		0.10520
##	84358402	0.10	030	0.13280	0.1980		0.10430
##	843786	0.12		0.17000	0.1578		0.08089
##		symmetry_mea	n fractal_	_dimension_mean			erimeter_se
##	842302	0.241	.9	0.07871	1.0950	0.9053	8.589
##	842517	0.181	.2	0.05667	0.5435	0.7339	3.398
##	84300903	0.206	9	0.05999	0.7456	0.7869	4.585
##	84348301	0.259		0.09744		1.1560	3.445
##	84358402	0.180	9	0.05883	0.7572	0.7813	5.438
##	843786	0.208	37	0.07613	0.3345	0.8902	2.217
##			thness_se	compactness_se		concave.po	oints_se
##	842302	153.40	0.006399	0.04904			0.01587
##	842517	74.08	0.005225	0.01308	0.01860		0.01340
##	84300903	94.03	0.006150	0.04006	0.03832		0.02058
##	84348301	27.23	0.009110	0.07458	0.05661		0.01867
	84358402	94.44	0.011490	0.02461			0.01885
##	843786	27.19	0.007510	0.03345			0.01137
##		symmetry_se fractal_dimension_se radius_worst texture_worst					
	842302	0.03003		0.006193	25.38	17.33	
	842517	0.01389		0.003532	24.99	23.41	
	84300903	0.02250		0.004571	23.57	25.53	
	84348301	0.05963		0.009208	14.91	26.50	
	84358402	0.01756		0.005115	22.54	16.67	
##	843786	0.02165		0.005082	15.47	23.75	
##		perimeter_wo	rst area_w	orst smoothnes	s_worst compac	tness_wors	st

```
## 842302
                      184.60
                                  2019.0
                                                    0.1622
                                                                        0.6656
## 842517
                                                                        0.1866
                      158.80
                                  1956.0
                                                    0.1238
## 84300903
                      152.50
                                  1709.0
                                                    0.1444
                                                                        0.4245
## 84348301
                                                    0.2098
                                                                        0.8663
                       98.87
                                   567.7
## 84358402
                      152.20
                                  1575.0
                                                    0.1374
                                                                        0.2050
## 843786
                      103.40
                                   741.6
                                                    0.1791
                                                                        0.5249
##
            concavity_worst concave.points_worst symmetry_worst
## 842302
                      0.7119
                                             0.2654
                                                             0.4601
## 842517
                      0.2416
                                             0.1860
                                                             0.2750
## 84300903
                      0.4504
                                             0.2430
                                                             0.3613
## 84348301
                      0.6869
                                             0.2575
                                                             0.6638
## 84358402
                      0.4000
                                             0.1625
                                                             0.2364
## 843786
                      0.5355
                                             0.1741
                                                             0.3985
##
            fractal_dimension_worst
## 842302
                              0.11890
## 842517
                              0.08902
## 84300903
                              0.08758
## 84348301
                              0.17300
## 84358402
                              0.07678
## 843786
                              0.12440
wisc.data <- wisc.df[,-1]</pre>
```

```
wisc.data <- wisc.df[,-1]
diagnosis <- factor(wisc.df$diagnosis, levels = c("B", "M"))
print(diagnosis)</pre>
```

```
##
 [38] В М М М М М М М В М В В В В М М В М М В В В В М В М М В В В В М В М М
## [112] B B B B B B M M M B M M B B B M M B M B M M B M M B B M B B M B B B B B M B
## [186] B M B B B M B B M M B M M M M B M M M B B M B B M B B M M M B B
## [556] B B B B B B B M M M M M B
## Levels: B M
```

### Q1: How many observations are in this dataset?

```
dim(wisc.data)
```

## [1] 569 30

It looks like there is 569 different observations.

#### Q2: How many of the observations have a malignant diagnosis?

#### table(diagnosis)

```
## diagnosis
## B M
## 357 212
```

There is 212 malignant observations

\*\*Q3: How many variables/features in the data are suffixed with \_mean?\*\*

```
length(grep("_mean", colnames(wisc.data)))
```

```
## [1] 10
```

10 columns have the term "\_mean" in them

Next: PCA

Check column means and standard deviations

#### colMeans(wisc.data)

```
##
               radius_mean
                                        texture_mean
                                                               perimeter_mean
##
              1.412729e+01
                                        1.928965e+01
                                                                 9.196903e+01
##
                  area_mean
                                     {\tt smoothness\_mean}
                                                             compactness_mean
##
              6.548891e+02
                                        9.636028e-02
                                                                  1.043410e-01
##
            concavity_mean
                                concave.points_mean
                                                                symmetry_mean
##
              8.879932e-02
                                        4.891915e-02
                                                                 1.811619e-01
##
    fractal_dimension_mean
                                           radius_se
                                                                    texture_se
##
              6.279761e-02
                                        4.051721e-01
                                                                  1.216853e+00
##
                                                                 smoothness_se
              perimeter_se
                                             area_se
##
              2.866059e+00
                                        4.033708e+01
                                                                 7.040979e-03
##
            compactness_se
                                        concavity_se
                                                            concave.points_se
              2.547814e-02
                                        3.189372e-02
                                                                  1.179614e-02
##
                                                                 radius_worst
##
               symmetry_se
                               fractal_dimension_se
              2.054230e-02
                                        3.794904e-03
                                                                 1.626919e+01
##
             texture_worst
                                     perimeter_worst
##
                                                                    area_worst
##
              2.567722e+01
                                        1.072612e+02
                                                                 8.805831e+02
##
          smoothness_worst
                                   compactness_worst
                                                              concavity_worst
                                                                  2.721885e-01
##
              1.323686e-01
                                        2.542650e-01
##
      concave.points_worst
                                      symmetry_worst fractal_dimension_worst
##
              1.146062e-01
                                        2.900756e-01
                                                                 8.394582e-02
```

#### apply(wisc.data,2,sd)

##	radius_mean	texture_mean	perimeter_mean
##	3.524049e+00	4.301036e+00	2.429898e+01
##	area_mean	smoothness_mean	compactness_mean
##	3.519141e+02	1.406413e-02	5.281276e-02
##	concavity_mean	concave.points_mean	symmetry_mean
##	7.971981e-02	3.880284e-02	2.741428e-02
##	fractal_dimension_mean	radius_se	texture_se

```
##
              7.060363e-03
                                        2.773127e-01
                                                                 5.516484e-01
##
              perimeter_se
                                                                smoothness_se
                                             area_se
                                        4.549101e+01
##
              2.021855e+00
                                                                 3.002518e-03
##
            compactness_se
                                        concavity_se
                                                            concave.points_se
##
              1.790818e-02
                                        3.018606e-02
                                                                 6.170285e-03
##
                               fractal dimension se
                                                                 radius worst
               symmetry se
##
              8.266372e-03
                                        2.646071e-03
                                                                 4.833242e+00
##
             texture_worst
                                     perimeter_worst
                                                                   area_worst
##
              6.146258e+00
                                        3.360254e+01
                                                                 5.693570e+02
##
          smoothness_worst
                                   compactness_worst
                                                              concavity_worst
##
              2.283243e-02
                                        1.573365e-01
                                                                 2.086243e-01
##
      concave.points_worst
                                      symmetry_worst fractal_dimension_worst
                                        6.186747e-02
##
              6.573234e-02
                                                                 1.806127e-02
```

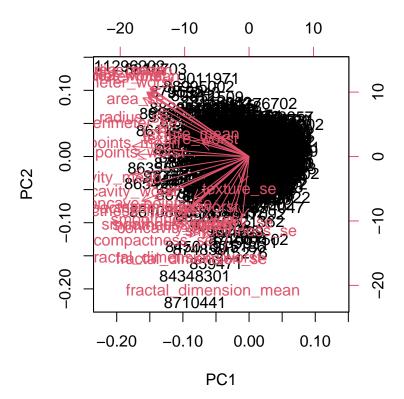
```
wisc.pr <- prcomp(wisc.data, scale. = TRUE)</pre>
```

#### summary(wisc.pr)

```
## Importance of components:
                                            PC3
                                                     PC4
                                                             PC5
                                                                     PC6
##
                             PC1
                                    PC2
                                                                             PC7
                          3.6444 2.3857 1.67867 1.40735 1.28403 1.09880 0.82172
## Standard deviation
## Proportion of Variance 0.4427 0.1897 0.09393 0.06602 0.05496 0.04025 0.02251
## Cumulative Proportion 0.4427 0.6324 0.72636 0.79239 0.84734 0.88759 0.91010
##
                              PC8
                                     PC9
                                            PC10
                                                    PC11
                                                            PC12
                                                                    PC13
                                                                            PC14
## Standard deviation
                          0.69037 0.6457 0.59219 0.5421 0.51104 0.49128 0.39624
## Proportion of Variance 0.01589 0.0139 0.01169 0.0098 0.00871 0.00805 0.00523
## Cumulative Proportion 0.92598 0.9399 0.95157 0.9614 0.97007 0.97812 0.98335
##
                                              PC17
                                                      PC18
                                                              PC19
                             PC15
                                     PC16
                                                                      PC20
## Standard deviation
                          0.30681 0.28260 0.24372 0.22939 0.22244 0.17652 0.1731
## Proportion of Variance 0.00314 0.00266 0.00198 0.00175 0.00165 0.00104 0.0010
## Cumulative Proportion 0.98649 0.98915 0.99113 0.99288 0.99453 0.99557 0.9966
                             PC22
                                     PC23
                                            PC24
                                                     PC25
                                                             PC26
##
                                                                     PC27
                                                                             PC28
## Standard deviation
                          0.16565 0.15602 0.1344 0.12442 0.09043 0.08307 0.03987
## Proportion of Variance 0.00091 0.00081 0.0006 0.00052 0.00027 0.00023 0.00005
## Cumulative Proportion
                          0.99749 0.99830 0.9989 0.99942 0.99969 0.99992 0.99997
##
                             PC29
                                     PC30
## Standard deviation
                          0.02736 0.01153
## Proportion of Variance 0.00002 0.00000
## Cumulative Proportion 1.00000 1.00000
```

- Q4: From your results, what proportion of the original variance is captured by the first principal components (PC1)? 44.27%
- Q5: How many principal components (PCs) are required to describe at least 70% of the original variance in the data? 3
- Q6: How many principal components (PCs) are required to describe at least 90% of the original variance in the data? 7

```
biplot(wisc.pr)
```



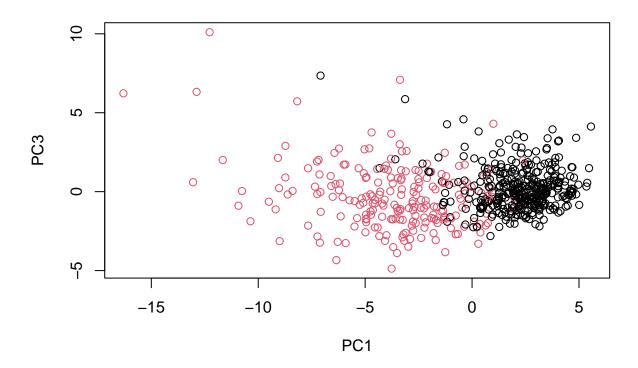
Q7: What stands out to you about this plot? Is it easy or difficult to understand? Why? Can't understand anything on the plot, impossible to read

```
plot( wisc.pr$x , col = diagnosis ,
     xlab = "PC1", ylab = "PC2")
```



Q8: Generate a similar plot for principal components  $\mathbf 1$  and  $\mathbf 3$ . What do you notice about these plots?

```
plot( wisc.pr$x[, c(1,3)] , col = diagnosis ,
    xlab = "PC1", ylab = "PC3")
```

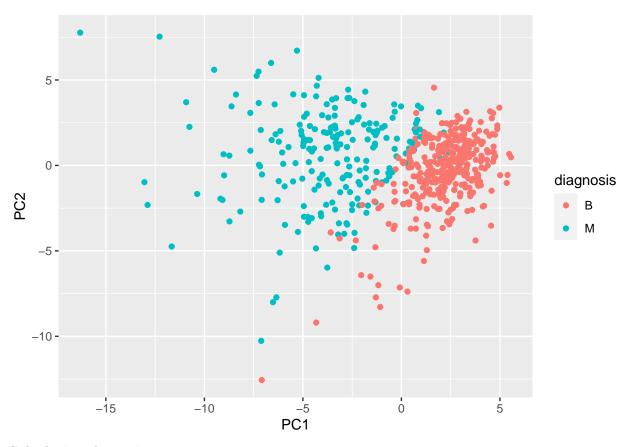


There seems to be two different cluster of cells, red dots(or malignant) and black dots (or benign)

### Creating ggplot for our data

```
df <- as.data.frame(wisc.pr$x)
df$diagnosis <- diagnosis</pre>
```

```
library(ggplot2)
ggplot(df) + aes(PC1, PC2, col=diagnosis) +
  geom_point()
```

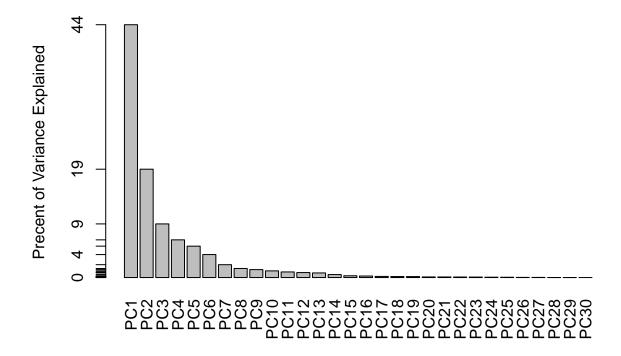


## Calculating the variance now

```
pr.var <- wisc.pr$sdev^2
head(pr.var)</pre>
```

**##** [1] 13.281608 5.691355 2.817949 1.980640 1.648731 1.207357





Q9: For the first principal component, what is the component of the loading vector (i.e. wisc.pr\$rotation[,1]) for the feature concave.points\_mean?

```
wisc.pr$rotation["concave.points_mean",1]
```

## [1] -0.2608538

Q10: What is the minimum number of principal components required to explain 80% of the variance of the data?

```
summary(wisc.pr)
```

```
## Importance of components:
##
                             PC1
                                    PC2
                                             PC3
                                                     PC4
                                                             PC5
                                                                     PC6
                                                                             PC7
## Standard deviation
                          3.6444 2.3857 1.67867 1.40735 1.28403 1.09880 0.82172
## Proportion of Variance 0.4427 0.1897 0.09393 0.06602 0.05496 0.04025 0.02251
## Cumulative Proportion 0.4427 0.6324 0.72636 0.79239 0.84734 0.88759 0.91010
                                                    PC11
                                                            PC12
##
                              PC8
                                     PC9
                                             PC10
                                                                    PC13
                                                                            PC14
## Standard deviation
                          0.69037 0.6457 0.59219 0.5421 0.51104 0.49128 0.39624
## Proportion of Variance 0.01589 0.0139 0.01169 0.0098 0.00871 0.00805 0.00523
## Cumulative Proportion 0.92598 0.9399 0.95157 0.9614 0.97007 0.97812 0.98335
##
                             PC15
                                     PC16
                                              PC17
                                                      PC18
                                                              PC19
                                                                      PC20
                          0.30681 0.28260 0.24372 0.22939 0.22244 0.17652 0.1731
## Standard deviation
## Proportion of Variance 0.00314 0.00266 0.00198 0.00175 0.00165 0.00104 0.0010
## Cumulative Proportion 0.98649 0.98915 0.99113 0.99288 0.99453 0.99557 0.9966
```

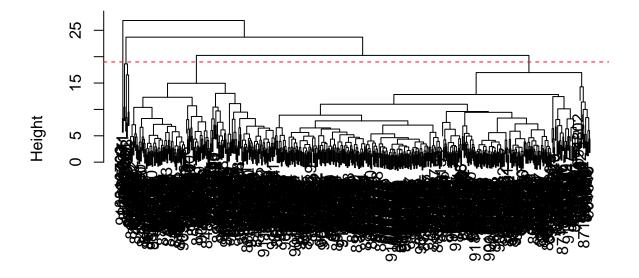
```
## Standard deviation 0.16565 0.15602 0.1344 0.12442 0.09043 0.08307 0.03987 ## Proportion of Variance 0.00091 0.00081 0.0006 0.00052 0.00027 0.00023 0.00005 ## Cumulative Proportion 0.99749 0.99830 0.9989 0.99942 0.99969 0.99992 0.99997 PC29 PC30 ## Standard deviation 0.02736 0.01153 ## Proportion of Variance 0.00002 0.00000 ## Cumulative Proportion 1.00000 1.00000
```

We need The first 5 PCs to get to at least 80%

Q11: Using the plot() and abline() functions, what is the height at which the clustering model has 4 clusters? *Hierarchical clustering* 

```
data.scaled <- scale(wisc.data)
data.dist <- dist(data.scaled)
wisc.hclust <- hclust(data.dist)
plot(wisc.hclust) +
abline(h=19, col="red", lty=2)</pre>
```

## **Cluster Dendrogram**



data.dist hclust (\*, "complete")

## integer(0)

Height 19 gives us 4 clusters.

```
wisc.hclust.clusters <- cutree(wisc.hclust, h=19)
table(wisc.hclust.clusters, diagnosis)</pre>
```

```
##
                         diagnosis
## wisc.hclust.clusters
                            В
##
                           12 165
##
                        2
                            2
                                5
##
                        3 343
                               40
##
                            0
                                2
```

Q12. Can you find a better cluster vs diagnoses match by cutting into a different number of clusters between 2 and 10?

```
wisc.hclust.clusters <- cutree(wisc.hclust, h=10)
table(wisc.hclust.clusters, diagnosis)</pre>
```

```
##
                           diagnosis
## wisc.hclust.clusters
                              В
                                  М
                              0
                                  24
##
                        1
                        2
                              0
                                  53
##
##
                        3
                              0
                                  3
##
                        4
                              0
                                 11
##
                             12
                        5
                                  46
##
                        6
                            100
                                  33
##
                        7
                              0
                                  14
##
                        8
                            197
                                   6
##
                        9
                              0
                                   5
##
                        10
                             19
                                   0
##
                        11
                             11
                                   0
##
                        12
                                   0
                              1
##
                        13
                             10
                                   0
##
                        14
                              0
                                   2
##
                        15
                              0
                                   6
##
                        16
                                   0
                              1
##
                        17
                              0
                                   6
##
                        18
                              4
                                   0
##
                        19
                                   2
##
                        20
                              0
                                   1
##
                        21
                              2
                                   0
```

```
wisc.hclust.clusters <- cutree(wisc.hclust, h=20)
table(wisc.hclust.clusters, diagnosis)</pre>
```

```
##
                        diagnosis
## wisc.hclust.clusters
                           В
                                М
##
                        1
                           12 165
##
                       2
                            2
                                5
##
                       3 343
                               40
##
                            0
                                2
```

```
wisc.hclust.clusters <- cutree(wisc.hclust, h=24)
table(wisc.hclust.clusters, diagnosis)</pre>
```

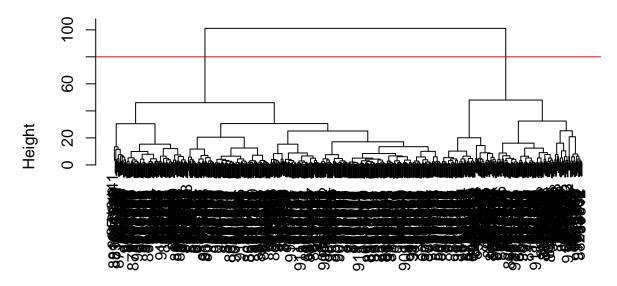
```
## diagnosis
## wisc.hclust.clusters B M
## 1 357 210
## 2 0 2
```

It seems that height 19-20 gives us the best clusters.

Q13. Which method gives your favorite results for the same data.dist dataset? Explain your reasoning.

```
wisc.pr.hclust <- hclust(dist(wisc.pr$x[,1:4]), method="ward.D2")
plot(wisc.pr.hclust)
abline(h=80, col="red")</pre>
```

# **Cluster Dendrogram**



dist(wisc.pr\$x[, 1:4]) hclust (\*, "ward.D2")

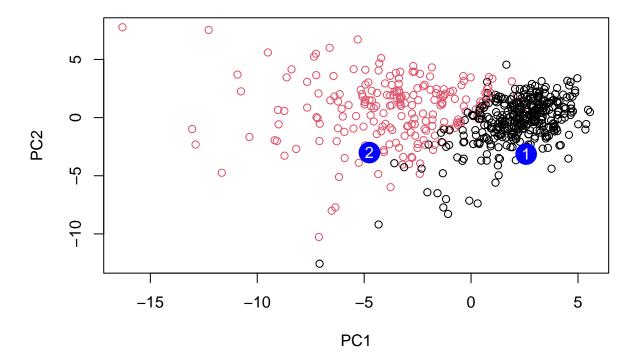
Q15: How well does the newly created model with four clusters separate out the two diagnoses?

```
grps <- cutree(wisc.pr.hclust, k=2)
table(grps)
## grps</pre>
```

## 1 2 ## 171 398 Comparing it to the expert M and B vector

```
table(diagnosis)
## diagnosis
##
     В
       M
## 357 212
We can do a cross-table by giving the table() function two inputs. (Called confusion table)
table(grps, diagnosis)
##
       diagnosis
## grps
          В
              Μ
          6 165
##
##
      2 351 47
Accuracy, essentially how many did we get correct?
(165+351)/nrow(wisc.data)
## [1] 0.9068541
Q17: Which of your analysis procedures resulted in a clustering model with the best specificity?
How about sensitivity?
Sensitivity
165/(165+47)
## [1] 0.7783019
Specificity
351/(351+47)
## [1] 0.8819095
url <- "new_samples.csv"</pre>
new <- read.csv(url)</pre>
npc <- predict(wisc.pr, newdata=new)</pre>
npc
              PC1
                         PC2
                                     PC3
                                                 PC4
                                                           PC5
                                                                       PC6
                                                                                   PC7
##
## [1,] 2.576616 -3.135913 1.3990492 -0.7631950 2.781648 -0.8150185 -0.3959098
## [2,] -4.754928 -3.009033 -0.1660946 -0.6052952 -1.140698 -1.2189945 0.8193031
##
               PC8
                          PC9
                                     PC10
                                                PC11
                                                          PC12
                                                                     PC13
## [1,] -0.2307350 0.1029569 -0.9272861 0.3411457 0.375921 0.1610764 1.187882
## [2,] -0.3307423 0.5281896 -0.4855301 0.7173233 -1.185917 0.5893856 0.303029
##
             PC15
                         PC16
                                      PC17
                                                   PC18
                                                                           PC20
                                                                PC19
```

```
## [1,] 0.3216974 -0.1743616 -0.07875393 -0.11207028 -0.08802955 -0.2495216
## [2,] 0.1299153 0.1448061 -0.40509706 0.06565549 0.25591230 -0.4289500
##
              PC21
                         PC22
                                               PC24
                                    PC23
                                                           PC25
## [1,] 0.1228233 0.09358453 0.08347651
                                         0.1223396
                                                    0.02124121 0.078884581
##
   [2,] -0.1224776 0.01732146 0.06316631 -0.2338618 -0.20755948 -0.009833238
##
                PC27
                            PC28
                                         PC29
                                                      PC30
## [1,] 0.220199544 -0.02946023 -0.015620933 0.005269029
## [2,] -0.001134152  0.09638361  0.002795349 -0.019015820
plot(wisc.pr$x[,1:2], col=diagnosis)
points(npc[,1], npc[,2], col="blue", pch=16, cex=3)
text(npc[,1], npc[,2], labels=c(1,2), col="white")
```



Q18. Which of these new patients should we prioritize for follow up based on your results? Patient number 2